Program

Challenges in Computational Homogeneous Catalysis

Långholmen - Stockholm
13-14 June 2013

Thursday 13 June

Session I: ***(Chair: Fahmi Himo)***

09.00 – 09.15 **Conference Opening**

09.15 – 09.50 **Jeremy Harvey**, University of Bristol, UK
Qualitative and Quantitative Insight into Reaction Mechanisms: Some Case Studies

09.50 – 10.25 **Stefan Grimme**, University of Bonn, Germany
Accurate Thermochemistry for Large Systems by Dispersion-Corrected Density Functional Theory

10.25 – 11.00 **Feliu Maseras**, Institute of Chemical Research of Catalonia, Spain
Enantioselective Catalysis: the Challenge of Small Energy Differences

11.00 – 11.30 **Coffee Break**

Session II: ***(Chair: Cristiana Di Valentin)***

11.30 – 12.05 **Michael Hall**, Texas A&M University, USA
Mechanism of the Reaction of Nickel bis(dithiolenes) with Alkenes

12.05 – 12.40 **Gregori Ujaque**, Autonomous University of Barcelona, Spain
Computational Challenges on the Suzuki-Miyaura Cross-Coupling Reaction

12.40 – 13.15 **Franziska Schoenebeck**, ETH Zurich, Switzerland
New Insights and Developments in Palladium Catalysis – a Combination of Theory and Experiment

13.15 – 14.45 **Lunch**

Session III: ***(Chair: Itai Panas)***

14.45 – 15.20 **Per-Ola Norrby**, University of Gothenburg, Sweden
On the Nature of Selectivity Determining Steps in Homogeneous Catalysis

15.20 – 15.55 **Satoshi Maeda**, Hokkaido University, Japan
Global Reaction Route Mapping Strategy for Systematic Prediction of Reaction Mechanisms in Homogeneous Catalysis

15.55 – 16.30 **Fahmi Himo**, Stockholm University, Sweden
Synergistic Catalysis Studied by a Combination of DFT and Kinetics Simulations

16.30 – 17.00 **Coffee Break**

Session IV: ***(Chair: Bo Durbeej)***

17.00 – 17.35 **Stuart MacGregor**, Heriot-Watt University, Scotland
Striking a Balance between C-H Activation and Functionalisation
17.35 – 18.10 **David Balcells**, University of Oslo, Norway
C-H Bond Strengthening and Deactivation in Transition Metal Complexes Revealed by First Principle Calculations
18.10 – 18.45 **Daniel Ess**, Brigham Young University, USA
Success and Failure of Quantitative/Qualitative Computations Interfacing with Experiment for the Design of Catalytic Bond Activation and Functionalization Reactions.

19.30 – **Dinner**

Friday 14 June

Session V: ***(Chair: Margareta Blomberg)***

09.00 – 09.35 **Christopher Cramer**, University of Minnesota, USA
Challenges Associated with Catalysts Undergoing Electron and Proton Transfers: Water-splitting Case Studies
09.35 – 10.10 **Per Siegbahn**, Stockholm University, Sweden
Modelling Redox Reactions where Electrons and Protons Enter or Leave: The Case of Water Oxidation
10.10 – 10.45 **Odile Eisenstein**, University of Montpellier, France
Modeling Amorphous Silica Grafted Schrock Olefin Metathesis Catalysts

10.45 – 11.15 **Coffee Break**

Session VI: ***(Chair: Ivan Rivalta)***

11.15 – 11.50 **Agustí Lledós**, Autonomous University of Barcelona, Spain
H-H Bond Activation: A Unified View
11.50 – 12.25 **Timofei Privalov**, Stockholm University, Sweden
Effects of Dynamics on the Reactivity of the Bimolecular Frustrated Lewis Pairs at Finite Temperature: the Splitting of H_2 and Involvement of Molecular Vibrations
12.25 – 13.00 **Evert Jan Meijer**, University of Amsterdam, The Netherlands
Modeling of Catalysis in Solution

13.00 – 14.30 **Lunch**

Session VII: ***(Chair: Mårten Ahlquist)***

14.30 – 15.05 **Walter Thiel**, Max-Planck-Institut für Kohlenforschung, Germany
Theoretical Studies of Rh-Catalyzed Asymmetric Hydrogenation

15.05 – 15.40 **Zhenyang Lin**, The Hong Kong University of Science & Technology, Hong Kong
Reactivities and Electronic Properties of Boryl Ligands

15.40 – 16.15 **Brian Yates**, University of Tasmania, Australia
Finely Balanced Mechanisms in Gold-Catalysed Reactions of Alcohols with Enynes

16.15 – Conference Closing

19.00 – 22.00 ***Conference Dinner on board S/S Stockholm to the Stockholm archipelago***